Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 338 °C

Global applicability domain: Inside

Local applicability domain index: 3.30e-01

Confidence level: 4.80e-01

Nearest Neighbors from the Training Set

Image not found
4-Nitrosodiphenylamine
Measured: 292
Predicted: 325

Image not found
4,4'-Methylenedianiline
Measured: 398
Predicted: 368

Image not found
1,2-Diphenylhydrazine
Measured: 309
Predicted: 350

Image not found
3,3'-Dimethylbenzidine
Measured: 339
Predicted: 371

Image not found
2-Methyl-5-nitro-1H-isoindole-1,3(2H)-dione
Measured: 361
Predicted: 323